Loop quantum modified gravity and its cosmological application

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A general nonperturvative loop quantization procedure for metric modified gravity is reviewed. As an example, this procedure is applied to scalar-tensor theories of gravity. The quantum kinematical framework of these theories is rigorously constructed. Both the Hamiltonian and master constraint operators are well defined and proposed to represent quantum dynamics of scalar-tensor theories. As an application to models, we set up the basic structure of loop quantum Brans-Dicke cosmology. The effective dynamical equations of loop quantum Brans-Dicke cosmology are also obtained, which lay a foundation for the phenomenological investigation to possible quantum gravity effects in cosmology.

PACS numbers: 04.60.Pp, 04.50.Kd

I. INTRODUCTION

As a background independent approach to quantize general relativity (GR), Loop quantum gravity(LQG) has been widely investigated in past 25 years [1–4]. Recently, this non-perturbative loop quantization procedure has been generalized to the metric $f(\mathcal{R})$ theories,[5, 6] Brsns-Dicke theory [7] and scalar-tensor theories[8]. The fact that this background-independent quantization method can be successfully extended to those modified theories of gravity relies on the key observation that these gravity theories can be reformulated into the connection dynamical formalism with a compact structure group. The purpose of this paper is to review how to get the connection dynamics of these modified gravity theories and how to quantize these theories by the nonperturbative loop quantization procedure.

In fact, modified gravity theories have recently received increased attention in issues related to“dark matter”, “dark energy” and non-trivial tests on gravity beyond GR. Since 1998, a series of independent and accurate observations, including type Ia supernova, cosmic microwave background anisotropy, weak gravity lens, baryon oscillation, etc, implied that our universe now is undergoing a period of accelerated expansion[9]. These results have caused the “dark energy” problem which is difficult to get a satisfactory interpretation within the framework of GR. Hence it is reasonable to consider the other possibility that GR is not a valid theory of gravity on a galactic or cosmological scale. Besides the well-known $f(\mathcal{R})$ theories, a competing relativistic theory of gravity was proposed by Brans and Dicke in 1961 [10], which is apparently compatible with Mach’s principle. To represent a varying “gravitational constant”, a scalar field is non-minimally coupled to the metric in Brans-Dicke theory. To interpret the observational results, the Brans-Dicke theory was generalized by Bergmann [11] and Wagoner [12] to more general scalar-tensor theories (STT). Moreover, scalar-tensor theories is also closely related to low energy effective actions of some string theory (see e.g. [13–15]). Since it can naturally lead to cosmological acceleration in certain models (see e.g. [16–19]), the scalar field in STT of gravity is expected to account for the “dark energy” problem. In addition, some models of STT of gravity may even account for the “dark matter” puzzle [20–22], which was revealed by the observed rotation curve of galaxy clusters.

There are infinite ways to modify GR. One may suspect which rules we should employed to do the modification. The decisive rule certainly comes from experiments. A large part of the non-trivial tests on gravity theory beyond GR is closely related to Einstein’s equivalence principle (EEP) [23]. There are many local experiments existed in solar-system supporting EEP, which implies that gravity should be described by metric theories. Indeed, STT are a class of representative metric theories, which have been received most attention. That is why we us it as an example to demonstrate our general loop quantization procedure for metric modified gravity theories. It is also worth noting that both the metric $f(\mathcal{R})$ theories and Palatini $f(\mathcal{R})$ theories are equivalent to certain special kinds of STT with the coupling parameter $\omega(\phi) = 0$ and $\omega(\phi) = -\frac{3}{2}$ respectively[24] Meanwhile the original Brans-Dicke theory is nothing but the particular case of constant ω and vanishing potential of ϕ. There are also some other types of modified metric gravity theories proposed in recent years, such as Horava-Lifshitz theory [25] and critical gravity [26] etc. Those theories are proposed based on the fact that GR is nonrenormalizable at perturbative level, while the introduction of higher order derivative terms might cure this problem. Thus it is quite interesting to see whether all those kind of metric theories of gravity could be quantized nonperturbatively.

The following sections of this paper are organized as follows. We first introduce a general scheme of loop quantization for metric modified gravity in section II. Then we use scalar-tensor theories as an example to show how our general quantization procedure works. In section III, we start with Hamiltonian analysis of STT. The coupling parameter of the STT naturally marks

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off two sectors of the theory. Based on the resulted connection dynamical formalism of STT, we then quantize the STT by extending the nonperturbative quantization procedure of LQG in section IV in the way similar to loop quantum $f(\mathcal{R})$ gravity [5, 6]. Nevertheless, the STT that we are considering are a much more general class of metric theories of gravity than metric $f(\mathcal{R})$ theories. The Hamiltonian constraint operators in both sectors of the theory can be well defined. To avoid possible quantum anomaly, master constraint program of STT are given in V. For cosmological application of above quantum gravity theories, we set up the basic structure of loop quantum Brans-Dicke cosmology and get its effective equations of motion in section VI. Finally some concluding remarks are given in the last section. Throughout the paper, we use Greek alphabet for spacetime indices, Latin alphabet a,b,c,..., for spatial indices, and i,j,k,..., for internal indices.

II. GENERAL SCHEME

In this section, we will first outline the general scheme of loop quantization for metric modified gravity[27]. Especially, we are mainly focus on 4-dimensional metric theories of gravity which is consistent with Einstein's equivalent principle. The prerequisite is that the theory which is under consideration should have a well-defined geometrical dynamics, which means a Hamiltonian formalism with 3-metric h_{ab} as one of configuration variables, and in addition the constraint algebra of this theory is first-class (perhaps after solving some second-class constraints). Without loss of generality, we can assume that the classical phase space of this theory consists of conjugate pairs (h_{ab}, p^{ab}) and (ϕ_B, π^B), where ϕ_B could be a scalar, vector, tensor or spinor field. Then the quantization scheme has the following recipe.

(i) To obtain a connection dynamical formalism, we first define a quantity $\tilde{K}_{ab}$ via

$$\tilde{K}_{ab} = \frac{2\kappa}{\sqrt{h}}\left(p_{ab} - \frac{1}{2}ph_{ab}\right). \tag{2.1}$$

Then we enlarge the phase space by transforming to the triad formulation as

$$(h_{ab}, p^{ab}) \Rightarrow (E^a_i \equiv \sqrt{h}h_{ab}e^a_i, \tilde{K}^i_a \equiv \tilde{K}_{ab}e^b_i). \tag{2.2}$$

Now we make a canonical transformation to connection formulation as:

$$(E^a_j, \tilde{K}^j_a) \Rightarrow (E^a_j, A^j_a \equiv \Gamma^j_a + \gamma\tilde{K}^j_a), \tag{2.3}$$

and due to symmetric property of p_{ab} we have $\tilde{K}_{a[i}E^a_{j]} = 0$. This will give us the Gaussian constraint, $\mathcal{D}_aE^a_i \equiv \partial_aE^a_i + \epsilon_{ijk}A^j_aE^a_k = 0$. Then it is straightforward to write all the constraints in terms of the new variables. (ii) For loop quantization, we first represent the fields (ϕ_B, π^B) via polymer-like representation, together with the LQG representation for the holonomy-flux algebra. Then the kinematical Hilbert space can be read as $\mathcal{H}_{\rm kin} := \mathcal{H}^{\rm gr}_{\rm kin} \otimes \mathcal{H}^{\phi}_{\rm kin}$. All the basic operators and geometrical operators could be well defined in this Hilbert space. We can solve the Gaussian and diffeomorphism constraints as in standard LQG. Then we would get the gauge and diffeomorphism invariant Hilbert spaceas: $\mathcal{H}_{\rm kin} \dashrightarrow \mathcal{H}_G \dashrightarrow \mathcal{H}_{Diff}$. In order to implement quantum dynamics, the Hamiltonian constraint operator may first be constructed at least in $\mathcal{H}_G$, although it usually could not be well defined in $\mathcal{H}_{Diff}$. Then the master constraint operator can be constructed in $\mathcal{H}_{Diff}$ by using the structure of the Hamiltonian operator. (iii) One may try to understand the physical Hilbert space by the direct integral decomposition of $\mathcal{H}_{Diff}$ with respect to the spectrum of the master constraint operator. (iv) One may also do certain semiclassical analysis in order to confirm the classical limits of the Hamiltonian and master constraint operators as well as the constraint algebra. The low energy physics is also expected in the analysis. (v) Finally, to complement above canonical approach, we can also try the covariant path integral (spinfoam) quantization.

It should be noted that the last three steps are still open issues in the loop quantization of GR. Thus in the following sections, we will take scalar-tensor theories as an example to carry out the steps (i) and (ii) in the above scheme of loop quantization for metric modified gravity.

III. HAMILTONIAN ANALYSIS OF SCALAR-TENSOR THEORIES

The most general action of STT reads

$$S(g) = \frac{1}{2\kappa}\int_\Sigma d^4x\sqrt{-g}\left[\phi\mathcal{R} - \frac{\omega(\phi)}{\phi}(\partial_\mu\phi)\partial^\mu\phi - 2\xi(\phi)\right] \tag{3.1}$$

where $\kappa = 8\pi G$, $\mathcal{R}$ denotes the scalar curvature of spacetime metric $g_{\mu\nu}$, and the coupling parameter $\omega(\phi)$ and potential $\xi(\phi)$ can be arbitrary functions of scalar field ϕ. Variations of the action (3.1) with respect to g_{ab} and ϕ respectively give us equations of

motion

$$\phi G_{\mu\nu} = \nabla_\mu \nabla_\nu \phi - g_{\mu\nu}\Box\phi + \frac{\omega(\phi)}{\phi}[(\partial_\mu\phi)\partial_\nu\phi - \frac{1}{2}g_{\mu\nu}(\nabla\phi)^2] - g_{\mu\nu}\xi(\phi), \tag{3.2}$$

$$\mathcal{R} + \frac{2\omega(\phi)}{\phi}\Box\phi - \frac{\omega(\phi)}{\phi^2}(\partial_\mu\phi)\partial^\mu\phi + \frac{\omega'(\phi)}{\phi}(\partial_\mu\phi)\partial^\mu\phi - 2\xi'(\phi) = 0, \tag{3.3}$$

where a prime over a letter denotes a derivative with respect to the argument, ∇_μ is the covariant derivative compatible with $g_{\mu\nu}$ and $\Box \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu$. By doing 3+1 decomposition of the spacetime, the four-dimensional (4d) scalar curvature can be expressed as

$$\mathcal{R} = K_{ab}K^{ab} - K^2 + R + \frac{2}{\sqrt{-g}}\partial_\mu(\sqrt{-g}n^\mu K) - \frac{2}{N\sqrt{h}}\partial_a(\sqrt{h}h^{ab}\partial_b N) \tag{3.4}$$

where K_{ab} is the extrinsic curvature of a spatial hypersurface Σ, $K \equiv K_{ab}h^{ab}$, R denotes the scalar curvature of the 3-metric h_{ab} induced on Σ, n^μ is the unit normal of Σ and N is the lapse function. By Legendre transformation, the momenta conjugate to the dynamical variables h_{ab} and ϕ are defined respectively as

$$p^{ab} = \frac{\partial\mathcal{L}}{\partial\dot{h}_{ab}} = \frac{\sqrt{h}}{2\kappa}[\phi(K^{ab} - Kh^{ab}) - \frac{h^{ab}}{N}(\dot{\phi} - N^c\partial_c\phi)], \tag{3.5}$$

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = -\frac{\sqrt{h}}{\kappa}(K - \frac{\omega(\phi)}{N\phi}(\dot{\phi} - N^c\partial_c\phi)), \tag{3.6}$$

where N^c is the shift vector. The combination of the trace of Eq. (3.5) and Eq. (3.6) gives

$$(3 + 2\omega(\phi))(\dot{\phi} - N^a\partial_a\phi) = \frac{2\kappa N}{\sqrt{h}}(\phi\pi - p). \tag{3.7}$$

It is easy to see from Eq. (3.7) that one extra constraint $S = p - \phi\pi = 0$ emerges when $\omega(\phi) = -\frac{3}{2}$. Hence it is natural to mark off two sectors of the theories by $\omega(\phi) \neq -\frac{3}{2}$ and $\omega(\phi) = -\frac{3}{2}$.

A. Sector of $\omega(\phi) \neq -3/2$

In the case of $\omega(\phi) \neq -3/2$, the Hamiltonian of STT can be derived as a liner combination of constraints as

$$H_{total} = \int_\Sigma d^3x(N^aV_a + NH), \tag{3.8}$$

where the smeared diffeomorphism and Hamiltonian constraints read respectively

$$V(\overrightarrow{N}) = \int_\Sigma d^3xN^aV_a = \int_\Sigma d^3xN^a\left(-2D^b(p_{ab}) + \pi\partial_a\phi\right), \tag{3.9}$$

$$\begin{aligned} H(N) &= \int_\Sigma d^3xNH \\ &= \int_\Sigma d^3xN\left[\frac{2\kappa}{\sqrt{h}}\left(\frac{p_{ab}p^{ab} - \frac{1}{2}p^2}{\phi} + \frac{(p-\phi\pi)^2}{2\phi(3+2\omega)}\right) + \frac{\sqrt{h}}{2\kappa}\left(-\phi R + \frac{\omega(\phi)}{\phi}(D_a\phi)D^a\phi + 2D_aD^a\phi + 2\xi(\phi)\right)\right]. \end{aligned} \tag{3.10}$$

By the symplectic structure

$$\begin{aligned} \{h_{ab}(x), p^{cd}(y)\} &= \delta_a^{(c}\delta_b^{d)}\delta^3(x,y), \\ \{\phi(x), \pi(y)\} &= \delta^3(x,y), \end{aligned} \tag{3.11}$$

lengthy but straightforward calculations show that the constraints (3.9) and (3.10) comprise a first-class system similar to GR as:

$$\begin{aligned} \{V(\overrightarrow{N}), V(\overrightarrow{N}')\} &= V([\overrightarrow{N}, \overrightarrow{N}']), \\ \{H(M), V(\overrightarrow{N})\} &= -H(\mathcal{L}_{\overrightarrow{N}}M), \\ \{H(N), H(M)\} &= V(ND^aM - MD^aN). \end{aligned} \tag{3.12}$$

We can show that the above Hamiltonian formalism of STT is equivalent to their Lagrangian formalism[8].

To obtain the connection dynamical formalism of the STT, following the general scheme mentioned in last section, we define

$$\tilde{K}^{ab} = \phi K^{ab} + \frac{h^{ab}}{2N}(\dot{\phi} - N^c\partial_c\phi) = \phi K^{ab} + \frac{h^{ab}}{(3+2\omega)\sqrt{h}}(\phi\pi - p). \tag{3.13}$$

Then we can introduce new canonical pairs $(E^a_i \equiv \sqrt{h}e^a_i, \tilde{K}^i_a \equiv \tilde{K}_{ab}e^b_i)$, where e^a_i is the triad such that $h_{ab}e^a_ie^b_j = \delta_{ij}$. Now the symplectic structure (3.11) can be got from the following Poisson brackets:

$$\begin{aligned} \{E^a_j(x), E^b_k(y)\} &= \{\tilde{K}^j_a(x), \tilde{K}^k_b(y)\} = 0, \\ \{\tilde{K}^j_a(x), E^b_k(y)\} &= \kappa\delta^b_a\delta^j_k\delta(x,y). \end{aligned} \tag{3.14}$$

Note that since we have $\tilde{K}^{ab} = \tilde{K}^{ba}$, there have an additional constraint:

$$G_{jk} \equiv \tilde{K}_{a[j}E^a_{k]} = 0. \tag{3.15}$$

Now we can make a second canonical transformation via defining:

$$A^i_a = \Gamma^i_a + \gamma\tilde{K}^i_a, \tag{3.16}$$

where Γ^i_a is the spin connection determined by E^a_i, and γ is a nonzero real number. It is easy to see that our new variable A^j_a coincides with the Ashtekar-Barbero connection [28, 29] in the special case $\phi = 1$. The Poisson brackets among the new variables read:

$$\begin{aligned} \{A^j_a(x), E^b_k(y)\} &= \gamma\kappa\delta^b_a\delta^j_k\delta(x,y), \\ \{A^i_a(x), A^j_b(y)\} &= 0, \quad \{E^a_j(x), E^b_k(y)\} = 0. \end{aligned} \tag{3.17}$$

Now the phase space of the STT consists of conjugate pairs (A^i_a, E^b_j) and (ϕ, π). Combining Eq.(3.15) with the compatibility condition:

$$\partial_a E^a_i + \epsilon_{ijk}\Gamma^j_a E^{ak} = 0, \tag{3.18}$$

the standard Gaussian constraint can be obtained as

$$\mathcal{G}_i = \mathscr{D}_a E^a_i \equiv \partial_a E^a_i + \epsilon_{ijk}A^j_a E^{ak}, \tag{3.19}$$

which justifies A^i_a as an $su(2)$-connection. It is worth noting that, had we let $\gamma = \pm i$, the (anti-)self-dual complex connection formalism would be obtained. The original vector and Hamiltonian constraints can be written in terms of new variables up to Gaussian constraint respectively as

$$V_a = \frac{1}{\kappa\gamma}F^i_{ab}E^b_i + \pi\partial_a\phi, \tag{3.20}$$

$$\begin{aligned} H &= \frac{\phi}{2\kappa}\left[F^j_{ab} - (\gamma^2 + \frac{1}{\phi^2})\varepsilon_{jmn}\tilde{K}^m_a\tilde{K}^n_b\right]\frac{\varepsilon_{jkl}E^a_kE^b_l}{\sqrt{h}} \\ &+ \frac{\kappa}{(3+2\omega(\phi))}\left(\frac{(\tilde{K}^i_aE^a_i)^2}{\kappa^2\phi\sqrt{h}} + 2\frac{(\tilde{K}^i_aE^a_i)\pi}{\kappa\sqrt{h}} + \frac{\pi^2\phi}{\sqrt{h}}\right) \\ &+ \frac{1}{\kappa}\left[\frac{\omega(\phi)}{2\phi}\sqrt{h}(D_a\phi)D^a\phi + \sqrt{h}D_aD^a\phi + \sqrt{h}\xi(\phi)\right], \end{aligned} \tag{3.21}$$

where $F^i_{ab} \equiv 2\partial_{[a}A^i_{b]} + \epsilon^i{}_{kl}A^k_aA^l_b$ is the curvature of A^i_a. The total Hamiltonian can be expressed as a linear combination

$$H_{total} = \int_\Sigma \Lambda^i\mathcal{G}_i + N^aV_a + NH. \tag{3.22}$$

It is easy to check that the smeared Gaussian constraint, $\mathcal{G}(\Lambda) := \int_\Sigma d^3x\Lambda^i(x)\mathcal{G}_i(x)$, generates $SU(2)$ gauge transformations on the phase space, while the smeared constraint, $\mathcal{V}(\overrightarrow{N}) := \int_\Sigma d^3xN^a(V_a - A^i_a\mathcal{G}_i)$, generates spatial diffeomorphism transformations

on the phase space. Together with the smeared Hamiltonian constraint $H(N) = \int_\Sigma d^3xNH$, we can show that the constraints algebra has the following form:

$$\begin{aligned}
\{\mathcal{G}(\Lambda), \mathcal{G}(\Lambda')\} &= \kappa\mathcal{G}([\Lambda, \Lambda']), &(3.23)\\
\{\mathcal{G}(\Lambda), \mathcal{V}(\overrightarrow{N})\} &= -\mathcal{G}(\mathcal{L}_{\overrightarrow{N}}\Lambda,), &(3.24)\\
\{\mathcal{G}(\Lambda), H(N)\} &= 0, &(3.25)\\
\{\mathcal{V}(\overrightarrow{N}), \mathcal{V}(\overrightarrow{N}')\} &= \mathcal{V}([\overrightarrow{N}, \overrightarrow{N}']), &(3.26)\\
\{\mathcal{V}(\overrightarrow{N}), H(M)\} &= H(\mathcal{L}_{\overrightarrow{N}}M), &(3.27)\\
\{H(N), H(M)\} &= \mathcal{V}(ND^aM - MD^aN)\\
&+ \mathcal{G}\Big((N\partial_aM - M\partial_aN)h^{ab}A_b\Big)\\
&- \frac{[E^aD_aN, E^bD_bM]^i}{\kappa h}\mathcal{G}_i\\
&- \gamma^2\frac{[E^aD_a(\phi N), E^bD_b(\phi M)]^i}{\kappa h}\mathcal{G}_i. &(3.28)
\end{aligned}$$

Here Eqs.(3.23-3.27) can be understand by the geometrical interpretations of $\mathcal{G}(\Lambda)$ and $\mathcal{V}(\overrightarrow{N})$. The detail calculation on the Poisson bracket (3.28) between the two smeared Hamiltonian constraints can be seen in the Appendix of [8]. Hence the constraints are of first class. Furthermore, the constraint algebra of GR can be recovered for the special case when $\phi = 1$. To summarize, the STT of gravity in the sector $\omega(\phi) \neq -3/2$ have already been cast into the $su(2)$-connection dynamical formalism. The resulted Hamiltonian structure is quite similar to metric $f(R)$ theories[6].

B. Sector of $\omega(\phi) = -3/2$

In the sector of $\omega(\phi) = -3/2$, Eq. (3.7) implies that there is an extra primary constraint $S = 0$, which we call "conformal" constraint. Hence, as pointed out in Ref.[30], the total Hamiltonian in this case can be expressed as a liner combination of constraints as

$$H_{total} = \int_\Sigma d^3x(N^aV_a + NH + \lambda S), \tag{3.29}$$

where the smeared diffeomorphism constraint $V(\overrightarrow{N})$ is as same as (3.9), while the Hamiltonian and conformal constraints read respectively

$$\begin{aligned}
H(N) &= \int_\Sigma d^3xNH\\
&= \int_\Sigma d^3xN\left[\frac{2\kappa}{\sqrt{h}}\left(\frac{p_{ab}p^{ab} - \frac{1}{2}p^2}{\phi}\right) + \frac{\sqrt{h}}{2\kappa}(-\phi R - \frac{3}{2\phi}(D_a\phi)D^a\phi + 2D_aD^a\phi + 2\xi(\phi))\right], &(3.30)\\
S(\lambda) &= \int_\Sigma d^3x\lambda S = \int_\Sigma d^3x\lambda(p - \phi\pi). &(3.31)
\end{aligned}$$

With the help of symplectic structure (3.11), straightforward calculations show that

$$\begin{aligned}
\{H(M), V(\overrightarrow{N})\} &= -H(\mathcal{L}_{\overrightarrow{N}}M), \quad \{S(\lambda), V(\overrightarrow{N})\} = -S(\mathcal{L}_{\overrightarrow{N}}\lambda), &(3.32)\\
\{H(N), H(M)\} &= V(ND^aM - MD^aN) + S(\frac{D_a\phi}{\phi}(ND^aM - MD^aN)), &(3.33)\\
\{S(\lambda), H(M)\} &= H(\frac{\lambda M}{2}) + \int_\Sigma N\lambda\sqrt{h}(-2\xi(\phi) + \phi\xi'(\phi)). &(3.34)
\end{aligned}$$

The Poisson bracket (3.34) implies that, we have to impose a secondary constraint in order to maintain the constraints S and H in the time evolution as

$$-2\xi(\phi) + \phi\xi'(\phi) = 0. \tag{3.35}$$

It is clear that this constraint is second-class, and hence one has to solve it. Here we consider the vacuum case where the solutions of Eq. (3.35) are either $\xi(\phi) = 0$ or $\xi(\phi) = C\phi^2$, where C is certain dimensional constant. Thus the consistency condition strongly

restricted the feasible STT in this sector to only two theories. As pointed out in Ref.[24], for these two theories, the action (3.1) is invariant under the following conformal transformation:

$$g_{\mu\nu} \to e^{\lambda} g_{\mu\nu}, \quad \phi \to e^{-\lambda}\phi. \tag{3.36}$$

Thus, besides diffeomorphism invariance, those two theories are also conformally invariant. Now in the resulted Hamiltonian formalism the constraints (V, H, S) form a first-class system. The following transformations on the phase space are generated by the conformal constraint

$$\{h_{ab}, S(\lambda)\} = \lambda h_{ab}, \quad \{P^{ab}, S(\lambda)\} = -\lambda P^{ab}, \tag{3.37}$$

$$\{\phi, S(\lambda)\} = -\lambda\phi, \quad \{\pi, S(\lambda)\} = \lambda\pi. \tag{3.38}$$

It is clear that the above transformations coincide with those of spacetime conformal transformations (3.36). Hence all constraints have clear physical meaning. Now the physical degrees of freedom of this special kind of STT are equal to those of GR because of the extra conformal constraint (3.31).

The connection-dynamical formalism for STT in this sector can also be obtained by the canonical transformations to the new variables (3.16). Then the total Hamiltonian can be expressed again as a linear combination

$$H_{total} = \int_\Sigma \Lambda^i \mathcal{G}_i + N^a V_a + NH + \lambda S, \tag{3.39}$$

where the Gaussian and diffeomorphism constraints keep the same form as Eqs. (3.19) and (3.20), while the Hamiltonian and the conformal constraints read respectively

$$\begin{aligned} H &= \frac{\phi}{2\kappa}\left[F^j_{ab} - (\gamma^2 + \frac{1}{\phi^2})\varepsilon_{jmn}\tilde{K}^m_a\tilde{K}^n_b\right]\frac{\varepsilon_{jkl}E^a_kE^b_l}{\sqrt{h}} \\ &+ \frac{1}{\kappa}\Big[-\frac{3}{4\phi}\sqrt{h}(D_a\phi)D^a\phi + \sqrt{h}D_aD^a\phi + \sqrt{h}\xi(\phi)\Big], \end{aligned} \tag{3.40}$$

$$S = \frac{1}{\kappa}\tilde{K}^i_aE^a_i - \pi\phi. \tag{3.41}$$

Now the constraints algebra in the connection formalism is closed as

$$\{\mathcal{G}(\Lambda), H(N)\} = 0, \tag{3.42}$$

$$\{\mathcal{G}(\Lambda), S(\lambda)\} = 0, \tag{3.43}$$

$$\{S(\lambda), H(M)\} = H(\frac{\lambda M}{2}), \tag{3.44}$$

$$\begin{aligned} \{H(N), H(M)\} &= \Big[\mathcal{V}(ND^aM - MD^aN) \\ &+ S(\frac{D_a\phi}{\phi}(ND^aM - MD^aN)) \\ &+ \mathcal{G}\Big((N\partial_aM - M\partial_aN)h^{ab}A_b\Big) \\ &- \frac{[E^aD_aN, E^bD_bM]^i}{\kappa h}\mathcal{G}_i \\ &- \gamma^2\frac{[E^aD_a(\phi N), E^bD_b(\phi M)]^i}{\kappa h}\mathcal{G}_i\Big]. \end{aligned} \tag{3.45}$$

It is easy to see that the Poisson brackets among the other constraints weakly equal to zero. Hence we have cast STT of gravity with $\omega(\phi) \neq -3/2$ into the $su(2)$-connection dynamical formalism.

IV. LOOP QUANTIZATION OF SCALAR-TENSOR THEORIES

Based on the connection dynamical formalism obtained in last section, the nonperturbative loop quantization procedure can be naturally extended to the STT. The kinematical structure of STT is as same as that of LQG coupled with a scalar field and $f(\mathcal{R})$ theories [5, 6]. The kinematical Hilbert space of the system is a direct product of the Hilbert space of geometry part and that of scalar field, $\mathcal{H}_{\rm kin} := \mathcal{H}^{\rm gr}_{\rm kin} \otimes \mathcal{H}^{\rm sc}_{\rm kin}$. An orthonormal basis of this Hilbert space is the so called spin-scalar-network basis, $T_{\alpha,X}(A,\phi) \equiv T_\alpha(A) \otimes T_X(\phi)$, over some graph $\alpha \cup X \subset \Sigma$, where α and X consist of finite number of curves and points in Σ

respectively. The basic operators of quantum STT are the quantum analogue of holonomies $h_e(A) = \mathcal{P}\exp\int_e A_a$ of a connection along edges $e \subset \Sigma$, densitized triads $E(S, f) := \int_S \epsilon_{abc} E^a_i f^i$ smeared over 2-surfaces, point holonomies $U_\lambda = \exp(i\lambda\phi(x))$[31], and scalar momenta $\pi(R) := \int_R d^3x\pi(x)$ smeared on 3-dimensional regions. It is worth noting that the spatial geometric operator, such as the area[32] , the volume[33] and the length[34, 35] operators, are still valid in $\mathcal{H}^{\rm gr}_{\rm kin}$ of quantum STT. As in LQG, it is natural to promote the Gaussian constraint $\mathcal{G}(\Lambda)$ as a well-defined operator[2, 4]. Then it's kernel is the internal gauge invariant Hilbert space $\mathcal{H}_G$ with gauge invariant spin-scalar-network basis. Since the diffeomorphisms of Σ act covariantly on the cylindrical functions in $\mathcal{H}_G$, the group averaging technique can be employed to solve the diffeomorphism constraint [3, 4, 6]. Hence the desired diffeomorphism and gauge invariant Hilbert space $\mathcal{H}_{Diff}$ for the STT can also be obtained[6, 8].

A. Sector of $\omega(\phi) \neq -3/2$

While the kinematical framework of LQG and polymer-like scalar field have been straight-forwardly extended to the STT, the nontrivial task in the case of $\omega(\phi) \neq -3/2$ is to implement the Hamiltonian constraint (3.21) at quantum level. In order to compare the Hamiltonian constraint of STT with that of metric $f(\mathcal{R})$ theories in connection formalism, we write Eq. (3.21) as $H(N) = \sum_{i=1}^{8} H_i$ in regular order. It is easy to see that the terms H_1, H_2, H_7, H_8 just keep the same form as those in $f(\mathcal{R})$ theories (see Eq.(39) in Ref.[6]), and the H_3, H_4, H_5 terms are also similar to the corresponding terms in $f(\mathcal{R})$ theories. Here the differences are only reflected by the coefficients as certain functions of ϕ. Now we come to the completely new term, $H_6 = \int_\Sigma d^3x N\frac{\omega(\phi)}{2\phi}\sqrt{h}(D_a\phi)D^a\phi$. This term is somehow like the kinetic term of a Klein-Gordon field which was dealt with in Ref.[36]. We can introduce the well-defined operators ϕ, ϕ^{-1} as in Ref. [6]. It is reasonable to believe that function $\omega(\phi)$ can also be quantized [6]. By the same regularization techniques as in Refs.[6, 36], we triangulate Σ in adaptation to some graph α underling a cylindrical function in $\mathcal{H}_{\rm kin}$ and reexpress connections by holonomies. The corresponding regulated operator acts on a basis vector $T_{\alpha,X}$ over some graph $\alpha \cup X$ as

$$\begin{aligned}
\hat{H}^{\varepsilon}_6 \cdot T_{\alpha,X} \;=\; & \lim_{\epsilon\to 0} \frac{2^{17} N(v)\hat{\omega}(\phi)}{3^6\gamma^4(i\lambda_0)^2(i\hbar)^4\kappa}\hat{\phi}^{-1}(v)\chi_\epsilon(v-v') \\
&\times \sum_{v\in\alpha(v)}\frac{1}{E(v)}\sum_{v(\Delta)=v}\epsilon(s_L s_M s_N)\epsilon^{LMN}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_L(\Delta_v)})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_L(\Delta_v)})) - \hat{U}_{\lambda_0}(\phi(s_{s_L(\Delta_v)}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_M(\Delta_v)}[\hat{h}^{-1}_{s_M(\Delta_v)}, (\hat{V}_{U^\epsilon_v})^{3/4}]\hat{h}_{s_N(\Delta_v)}[\hat{h}^{-1}_{s_N(\Delta_v)}, (\hat{V}_{U^\epsilon_v})^{3/4}]) \\
&\times \sum_{v'\in\alpha(v)}\frac{1}{E(v')}\sum_{v(\Delta')=v'}\epsilon(s_I s_J s_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta_{v'})})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta_{v'})})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta_{v'})}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_J(\Delta_{v'})}[\hat{h}^{-1}_{s_J(\Delta_{v'})}, (\hat{V}_{U^\epsilon_{v'}})^{3/4}]\hat{h}_{s_K(\Delta_{v'})}[\hat{h}^{-1}_{s_K(\Delta_{v'})}, (\hat{V}_{U^\epsilon_{v'}})^{3/4}]) \cdot T_{\alpha,X}. \qquad (4.1)
\end{aligned}$$

We refer to [6] for the meaning of notations in Eq.(4.1). It is easy to see that the action of $\hat{H}^{\varepsilon}_6$ on $T_{\alpha,X}$ is graph changing. It adds a finite number of vertices at $t(s_I(v)) = \varepsilon$ for edges $e_I(t)$ starting from each high-valent vertex of α. As a result, the family of operators $\hat{H}^{\varepsilon}_6(N)$ fails to be weakly convergent when $\varepsilon \to 0$. However, due to the diffeomorphism covariant properties of the triangulation, the limit operator can be well defined via the so-called uniform Rovelli-Smolin topology induced by diffeomorphism-invariant states Φ_{Diff} as:

$$\Phi_{Diff}(\hat{H}_6 \cdot T_{\alpha,X}) = \lim_{\varepsilon\to 0}\langle\Phi_{Diff}|\hat{H}^{\varepsilon}_6|T_{\alpha,X}\rangle. \qquad (4.2)$$

It is obviously that the limit is independent of ε. Hence both the regulators ϵ and ε can be removed. We then have

$$
\begin{aligned}
\hat{H}_6 \cdot T_{\alpha,X} &= \sum_{v\in V(\alpha)} \frac{2^{17} N(v)\hat{\omega}(\phi)}{3^6\gamma^4(i\lambda_0)^2(i\hbar)^4\kappa E^2(v)}\hat{\phi}^{-1}(v) \\
&\times \sum_{v(\Delta)=v(\Delta')=v} \epsilon(s_L s_M s_N)\epsilon^{LMN}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_L(\Delta)})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_L(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_L(\Delta)}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)}, (\hat{V}_v)^{3/4}]\hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)}, (\hat{V}_v)^{3/4}]) \\
&\times \epsilon(s_I s_J s_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta')})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta')})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_J(\Delta')}[\hat{h}^{-1}_{s_J(\Delta')}, (\hat{V}_v)^{3/4}]\hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')}, (\hat{V}_v)^{3/4}]) \cdot T_{\alpha,X}.
\end{aligned} \tag{4.3}
$$

In order to simplify the expression, we introduce $f(\phi) = \frac{1}{3+2\omega(\phi)}$ for the other terms containing it in $H(N)$, which can also be promoted to a well-defined operator $\hat{f}(\phi)$. Hence, the terms H_3, H_4 and H_5 can be quantized as

$$
\begin{aligned}
\hat{H}_3 \cdot T_{\alpha,X} &= \sum_{v\in V(\alpha)} \frac{4N(v)\hat{f}(\phi(v))}{\gamma^3(i\hbar)^2\kappa}\hat{\phi}^{-1}(v) \\
&\times [\hat{H}^E(1), \sqrt{\hat{V}_v}][\hat{H}^E(1), \sqrt{\hat{V}_v}] \cdot T_{\alpha,X},
\end{aligned} \tag{4.4}
$$

$$
\begin{aligned}
\hat{H}_4 \cdot T_{\alpha,X} &= -\sum_{v\in V(\alpha)\cap X} \frac{2^{20} N(v)\hat{f}(\phi(v))}{3^5\gamma^6(i\hbar)^6 E^2(v)}\hat{\pi}(v) \\
&\times \sum_{v(\Delta)=v(\Delta')=v} \mathrm{Tr}(\tau_i \hat{h}_{s_L(\Delta)}[\hat{h}^{-1}_{s_L(\Delta)}, \hat{\tilde{K}}]) \\
&\times \epsilon(s_L s_M s_N)\epsilon^{LMN} \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)}, (\hat{V}_v)^{3/4}]\hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)}, (\hat{V}_v)^{3/4}]) \\
&\times \epsilon(s_I s_J s_K)\epsilon^{IJK} \\
&\times \mathrm{Tr}(\hat{h}_{s_I(\Delta')}[\hat{h}^{-1}_{s_I(\Delta')}, (\hat{V}_v)^{1/2}]\hat{h}_{s_J(\Delta')}[\hat{h}^{-1}_{s_J(\Delta')}, (\hat{V}_v)^{1/2}] \\
&\times \hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,X},
\end{aligned} \tag{4.5}
$$

$$
\begin{aligned}
\hat{H}_5 \cdot T_{\alpha,X} &= \sum_{v\in V(\alpha)\cap X} \frac{2^{18}\kappa N(v)\hat{f}(\phi(v))}{3^4\gamma^6(i\hbar)^6 E^2(v)}\hat{\phi}(v)\hat{\pi}(v)\hat{\pi}(v) \\
&\times \sum_{v(\Delta)=v(\Delta')=v} \epsilon(s_I s_J s_K)\epsilon^{IJK} \\
&\times \mathrm{Tr}(\hat{h}_{s_I(\Delta)}[\hat{h}^{-1}_{s_I(\Delta)}, (\hat{V}_v)^{1/2}]\hat{h}_{s_J(\Delta)}[\hat{h}^{-1}_{s_J(\Delta)}, (\hat{V}_v)^{1/2}] \\
&\times \hat{h}_{s_K(\Delta)}[\hat{h}^{-1}_{s_K(\Delta)}, (\hat{V}_v)^{1/2}]) \\
&\times \epsilon(s_L s_M s_N)\epsilon^{LMN} \\
&\times \mathrm{Tr}(\hat{h}_{s_L(\Delta')}[\hat{h}^{-1}_{s_L(\Delta')}, (\hat{V}_v)^{1/2}]\hat{h}_{s_M(\Delta')}[\hat{h}^{-1}_{s_M(\Delta')}, (\hat{V}_v)^{1/2}] \\
&\times \hat{h}_{s_N(\Delta')}[\hat{h}^{-1}_{s_N(\Delta')}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,X}.
\end{aligned} \tag{4.6}
$$

While the H_7 and H_8 terms keep the same form as in $f(\mathcal{R})$ theory, which read respectively

$$
\begin{aligned}
\hat{H}_7 \cdot T_{\alpha,X} &= \sum_{v\in V(\alpha)} \frac{2^7 N(v)}{3\gamma^2 i\lambda_0 (i\hbar)^2 \kappa E(v)} \\
&\times \sum_{e(0)=v} X^i_e \sum_{v(\Delta)=v} \epsilon(s_I s_J s_K)\epsilon^{IJK} \\
&\times \hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta)}))[\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta)}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_J(\Delta)})[\hat{h}^{-1}_{s_J(\Delta)}, (\hat{V}_v)^{1/2}] \\
&\times \hat{h}_{s_K(\Delta)}[\hat{h}^{-1}_{s_K(\Delta)}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,X},
\end{aligned} \tag{4.7}
$$

$$
\hat{H}_8 \cdot T_{\alpha,X} = \frac{1}{\kappa} \sum_{v\in V(\alpha)} N(v)\hat{\xi}(\phi(v))\hat{V}_v \cdot T_{\alpha,X}. \tag{4.8}
$$

Here the action of the volume operator $\hat{V}$ on a spin-network basis vector $T_\alpha(A)$ over a graph α can be factorized as

$$
\hat{V} \cdot T_\alpha = \sum_{v\in V(\alpha)} \hat{V}_v \cdot T_\alpha. \tag{4.9}
$$

Therefore, the total Hamiltonian constraint in this sector has been quantized as a well-defined operator $\hat{H}(N) = \sum_{i=1}^{8} \hat{H}_i$ in $\mathcal{H}_{\text{kin}}$. It is easy to see that $\hat{H}(N)$ is internal gauge invariant and diffeomorphism covariant. Hence it is at least well defined in the gauge invariant Hilbert space $\mathcal{H}_G$. However, it is difficult to define $\hat{H}(N)$ directly on $\mathcal{H}_{Diff}$. Moreover, as in $f(R)$ theories, the constraint algebra of STT do not form a Lie algebra. This might lead to quantum anomaly after quantization.

B. Sector of $\omega(\phi) = -3/2$

In the special case of $\omega(\phi) = -3/2$, the smeared version $S(\lambda)$ of the extra conformal constraint (3.41) has to be promoted as a well-defined operator. Note that both ϕ and $\pi(R)$ are already well-defined operators. We can use the following classical identity to quantize the conformal constraint $S(\lambda)$,

$$
\tilde{K} \equiv \int_\Sigma d^3x \tilde{K}^i_a E^a_i = \gamma^{-\frac{3}{2}}\{H^E(1), V\} \tag{4.10}
$$

where the Euclidean scalar constraint $H^E(1)$ by definition was:

$$
H^E(1) = \frac{1}{2\kappa}\int_\Sigma d^3x F^j_{ab} \frac{\varepsilon_{jkl}E^a_k E^b_l}{\sqrt{h}}. \tag{4.11}
$$

Both H^E and the volume V have been quantized in LQG. Now it is easy to promote $S(\lambda)$ as a well-defined operator, and its action on a given basis vector $T_{\alpha,X} \in \mathcal{H}_{\text{kin}}$ reads

$$
\hat{S}(\lambda) \cdot T_{\alpha,X} = \left(\sum_{v\in V(\alpha)} \frac{\lambda(v)}{\gamma^{3/2}\kappa(i\hbar)} [\hat{H}^E(1), \hat{V}_v] - \sum_{x\in X} \lambda(x)\hat{\phi}(x)\hat{\pi}(x) \right) \cdot T_{\alpha,X}. \tag{4.12}
$$

It is clear that $\hat{S}(\lambda)$ is internal gauge invariant, diffeomorphism covariant and graph-changing. Hence it is well defined in $\mathcal{H}_G$. The Hamiltonian constraint operator in this sector is similar to that in the sector of $\omega(\phi) \neq -3/2$. The difference is that now $\omega(\phi) = -3/2$. Hence we write Eq. (3.40) as $H(N) = \sum_{i=1}^{5} H_i$ in regular order. It is easy to see that the terms H_1, H_2, H_4, H_5 just

keep the same form as those in last subsection, while the quantized version of H_3 is

$$\begin{aligned}
\hat{H}_3 \cdot T_{\alpha,X} &= -\sum_{v\in V(\alpha)} \frac{2^{16}N(v)}{3^5\gamma^4(i\lambda_0)^2(i\hbar)^4\kappa E^2(v)}\hat{\phi}^{-1}(v) \\
&\times \sum_{v(\Delta)=v(\Delta')=v} \epsilon(s_L s_M s_N)\epsilon^{LMN}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_L(\Delta)})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_L(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_L(\Delta)}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)}, (\hat{V}_v)^{3/4}]\hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)}, (\hat{V}_v)^{3/4}]) \\
&\times \epsilon(s_I s_J s_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta')})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta')})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')}))] \\
&\times \mathrm{Tr}(\tau_i \hat{h}_{s_J(\Delta')})[\hat{h}^{-1}_{s_J(\Delta')}, (\hat{V}_v)^{3/4}]\hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')}, (\hat{V}_v)^{3/4}]) \cdot T_{\alpha,X}.
\end{aligned} \tag{4.13}$$

Hence the total Hamiltonian constraint operator $\hat{H}(N) = \sum_{i=1}^{5} \hat{H}_i$ now is also well defined in $\mathcal{H}_G$.

V. MASTER CONSTRAINT

In order to find the physical Hilbert space and avoid possible quantum anomaly, master constraint programme was first introduced into LQG by Thiemann in his seminal paper[37]. The master constraint can be employed to implement the Hamiltonian constraint. This programme can also be generalized to the above quantum STT.

A. Sector of $\omega(\phi) \neq -3/2$

In the sector of $\omega(\phi) \neq -3/2$, by definition, the master constraint of the STT classically reads

$$\mathcal{M} := \frac{1}{2}\int_\Sigma d^3x \frac{|H(x)|^2}{\sqrt{h}}, \tag{5.1}$$

where the expression of Hamiltonian constraint $H(x)$ is given by Eq. (3.21). The master constraint can be regulated by a point-splitting strategy [38] as:

$$\mathcal{M}^\epsilon = \frac{1}{2}\int_\Sigma d^3y \int_\Sigma d^3x \chi_\epsilon(x-y)\frac{H(x)}{\sqrt{V_{U^\epsilon_x}}}\frac{H(y)}{\sqrt{V_{U^\epsilon_y}}}. \tag{5.2}$$

Introducing a partition $\mathcal{P}$ of the 3-manifold Σ into cells C, we can get an operator $\hat{H}^\varepsilon_{C,\beta}$ acting on the internal gauge-invariant spin-scalar-network basis $T_{s,c}$ in $\mathcal{H}_G$ via a state-dependent triangulation,

$$\hat{H}^\varepsilon_{C,\alpha} \cdot T_{s,c} = \sum_{v\in V(\alpha)} \chi_C(v)\hat{H}^\varepsilon_v \cdot T_{s,c}, \tag{5.3}$$

where χ_C is the characteristic function over C, α denotes the underlying graph of the spin-network state T_s, and

$$\hat{H}^\varepsilon_v = \sum_{v(\Delta)=v} \hat{H}^{\varepsilon,\Delta}_{GR,v} + \sum_{i=3}^{8} \hat{H}^\varepsilon_{i,v}, \tag{5.4}$$

with

$$\begin{aligned}
\hat{H}^\varepsilon_{3,v} &= \frac{16\hat{f}(\phi(v))}{\gamma^3(i\hbar)^2\kappa}\hat{\phi}^{-1}(v) \\
&\times [\hat{H}^E(1), (\hat{V}_{U^\epsilon_v})^{1/4}][\hat{H}^E(1), (\hat{V}_{U^\epsilon_v})^{1/4}],
\end{aligned} \tag{5.5}$$

$$\begin{aligned}
\hat{H}^{\varepsilon}_{4,v} &= -\sum_{v(\Delta)=v(\Delta')=v(X)=v} \frac{2^{18}\hat{f}(\phi(v))}{3^3\gamma^6(i\hbar)^6E^2(v)}\hat{\pi}(v) \\
&\times \mathrm{Tr}(\tau_i\hat{h}_{s_L(\Delta)}[\hat{h}^{-1}_{s_L(\Delta)},\hat{\tilde{K}}]) \\
&\times \epsilon(s_Ls_Ms_N)\epsilon^{LMN}\mathrm{Tr}(\tau_i\hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/2}] \\
&\times \hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/2}]) \\
&\times \epsilon(s_Is_Js_K)\epsilon^{IJK}\mathrm{Tr}(\hat{h}_{s_I(\Delta')}[\hat{h}^{-1}_{s_I(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/2}] \\
&\times \hat{h}_{s_J(\Delta')}[\hat{h}^{-1}_{s_J(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/2}] \\
&\times \hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/2}]),
\end{aligned} \tag{5.6}$$

$$\begin{aligned}
\hat{H}^{\varepsilon}_{5,v} &= \sum_{v(\Delta)=v(\Delta')=v(X)=v} \frac{2^{20}\kappa\hat{f}(\phi(v))}{3^4\gamma^6(i\hbar)^6E^2(v)}\hat{\phi}(v)\hat{\pi}(v)\hat{\pi}(v) \\
&\times \epsilon(s_Is_Js_K)\epsilon^{IJK}\mathrm{Tr}(\hat{h}_{s_I(\Delta)}[\hat{h}^{-1}_{s_I(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/4}] \\
&\times \hat{h}_{s_J(\Delta)}[\hat{h}^{-1}_{s_J(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/2}] \\
&\times \hat{h}_{s_K(\Delta)}[\hat{h}^{-1}_{s_K(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/2}]) \\
&\times \epsilon(s_Ls_Ms_N)\epsilon^{LMN}\mathrm{Tr}(\hat{h}_{s_L(\Delta')}[\hat{h}^{-1}_{s_L(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/4}] \\
&\times \hat{h}_{s_M(\Delta')}[\hat{h}^{-1}_{s_M(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/2}] \\
&\times \hat{h}_{s_N(\Delta')}[\hat{h}^{-1}_{s_N(\Delta')},(\hat{V}_{U^\epsilon_v})^{1/2}]),
\end{aligned} \tag{5.7}$$

$$\begin{aligned}
\hat{H}^{\varepsilon}_{6,v} &= \sum_{v(\Delta)=v(\Delta')=v} \frac{2^{15}\hat{\omega}(\phi)}{3^4\gamma^4(i\lambda_0)^2(i\hbar)^4\kappa E^2(v)}\hat{\phi}^{-1}(v) \\
&\times \epsilon(s_Ls_Ms_N)\epsilon^{LMN}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_L(\Delta)})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_L(\Delta)}))-\hat{U}_{\lambda_0}(\phi(s_{s_L(\Delta)}))] \\
&\times \mathrm{Tr}(\tau_i\hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)},(\hat{V}_v)^{1/2}]\hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)},(\hat{V}_v)^{3/4}]) \\
&\times \epsilon(s_Is_Js_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta')})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta')}))-\hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')}))] \\
&\times \mathrm{Tr}(\tau_i\hat{h}_{s_J(\Delta')}[\hat{h}^{-1}_{s_J(\Delta')},(\hat{V}_v)^{1/2}]\hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')},(\hat{V}_v)^{3/4}]),
\end{aligned} \tag{5.8}$$

$$\begin{aligned}
\hat{H}^{\varepsilon}_{7,v} &= \frac{2^9}{3\gamma^2 i\lambda_0(i\hbar)^2\kappa E(v)} \\
&\times \sum_{e(0)=v} X^i_e \sum_{v(\Delta)=v} \\
&\times \epsilon(s_Is_Js_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta)})) \\
&\times [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta)}))-\hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta)}))] \\
&\times \mathrm{Tr}(\tau_i\hat{h}_{s_J(\Delta)}[\hat{h}^{-1}_{s_J(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/4}] \\
&\times \hat{h}_{s_K(\Delta)}[\hat{h}^{-1}_{s_K(\Delta)},(\hat{V}_{U^\epsilon_v})^{1/4}]),
\end{aligned} \tag{5.9}$$

$$\hat{H}^{\varepsilon}_{8,v} = \frac{1}{\kappa}\hat{\xi}(\phi(v))\sqrt{\hat{V}_{U^\epsilon_v}}; \tag{5.10}$$

Here $\hat{H}^{\varepsilon,\Delta}_{GR,v}$ keeps the same form as the corresponding terms in [6]. Note that the family of operators $\hat{H}^{\varepsilon}_{C,\alpha}$ are cylindrically consistent up to diffeomorphism. Thus the inductive limit operator $\hat{H}_C$ is densely defined in $\mathcal{H}_G$ by the uniform Rovelli-Smolin topology. Hence we could define master constraint operator $\hat{\mathcal{M}}$ acting on a diffeomorphism invariant state as

$$(\hat{\mathcal{M}}\Phi_{Diff})T_{s,c} = \lim_{\mathcal{P}\to\Sigma,\varepsilon,\varepsilon'\to 0}\Phi_{Diff}[\frac{1}{2}\sum_{c\in\mathcal{P}}\hat{H}^{\varepsilon}_C(\hat{H}^{\varepsilon'}_C)^{\dagger}T_{s,c}]. \tag{5.11}$$

Note that although the quantitative actions are different, our construction of $\hat{\mathcal{M}}$ is qualitatively similar to those in [6, 36]. Similar methods in [6, 36] can be used here to prove that $\hat{\mathcal{M}}$ is a positive and symmetric operator in $\mathcal{H}_{Diff}$. Hence it admits a unique self-adjoint Friedrichs extension. It is then possible obtaining the physical Hilbert space of the quantum STT of this sector by the direct integral decomposition of $\mathcal{H}_{Diff}$ with respect to $\hat{\mathcal{M}}$.

B. Sector of $\omega(\phi) = -3/2$

In the case of $\omega(\phi) = -3/2$, both the implementation of the Hamiltonian constraint and the implementation of the conformal constraint need to employ the master constraint programme. We then define the master constraint for this sector as

$$\mathcal{M} := \frac{1}{2}\int_\Sigma d^3x \frac{|H(x)|^2 + |S(x)|^2}{\sqrt{h}}, \tag{5.12}$$

where the expressions of Hamiltonian constraint $H(x)$ and the conformal constraint $S(x)$ are given by Eqs. (3.40) and (3.41) respectively. It is clear that

$$\mathcal{M} = 0 \Leftrightarrow H(N) = 0 \quad and \quad S(\lambda) = 0 \quad \forall N(x), \lambda(x). \tag{5.13}$$

Now the constraints form a Lie algebra. The master constraint can be regulated by a point-splitting strategy as:

$$\mathcal{M}^\epsilon = \frac{1}{2}\int_\Sigma d^3y \int_\Sigma d^3x \chi_\epsilon(x-y) \frac{H(x)H(y) + S(x)S(y)}{\sqrt{V_{U^\epsilon_x}}\sqrt{V_{U^\epsilon_y}}}. \tag{5.14}$$

Introducing a partition $\mathcal{P}$ of the 3-manifold Σ into cells C, we get an operator $\hat{H}^\varepsilon_{C,\beta}$ acting on spin-scalar-network basis $T_{s,c}$ in $\mathcal{H}_G$ by a state-dependent triangulation as Eq. (5.3). Here, note that $\hat{H}^\varepsilon_v$ has less terms than in Eq. (5.3) as

$$\hat{H}^\varepsilon_v = \sum_{v(\Delta)=v} \hat{H}^{\varepsilon,\Delta}_{GR,v} + \sum_{i=3}^{5} \hat{H}^\varepsilon_{i,v}, \tag{5.15}$$

where

$$\begin{aligned}
\hat{H}^\varepsilon_{3,v} &= -\sum_{v(\Delta)=v(\Delta')=v} \frac{2^{14}}{3^3\gamma^4(i\lambda_0)^2(i\hbar)^4\kappa E^2(v)}\hat{\phi}^{-1}(v)\\
&\times\ \epsilon(s_L s_M s_N)\epsilon^{LMN}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_L(\Delta)}))\\
&\times\ [\hat{U}_{\lambda_0}(\phi(t_{s_L(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_L(\Delta)}))]\\
&\times\ \mathrm{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}^{-1}_{s_M(\Delta)}, (\hat{V}_v)^{1/2}]\hat{h}_{s_N(\Delta)}[\hat{h}^{-1}_{s_N(\Delta)}, (\hat{V}_v)^{3/4}])\\
&\times\ \epsilon(s_I s_J s_K)\epsilon^{IJK}\hat{U}^{-1}_{\lambda_0}(\phi(s_{s_I(\Delta')}))\\
&\times\ [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta')})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')}))]\\
&\times\ \mathrm{Tr}(\tau_i \hat{h}_{s_J(\Delta')}[\hat{h}^{-1}_{s_J(\Delta')}, (\hat{V}_v)^{1/2}]\hat{h}_{s_K(\Delta')}[\hat{h}^{-1}_{s_K(\Delta')}, (\hat{V}_v)^{3/4}]),
\end{aligned} \tag{5.16}$$

and $H^\varepsilon_{4,v}$ and $H^\varepsilon_{5,v}$ keep the same form as the corresponding terms in the sector of $\omega(\phi) \neq -3/2$. The operator corresponding to the conformal constraint can be defined in a similar way,

$$\hat{S}^\varepsilon_{C,\alpha} \cdot T_{s,c} = \sum_{v\in V(\alpha)} \chi_C(v)\hat{S}^\varepsilon_v \cdot T_{s,c}, \tag{5.17}$$

where

$$\hat{S}^\varepsilon_v = \hat{S}^\varepsilon_{1,v} + \hat{S}^\varepsilon_{2,v}, \tag{5.18}$$

with

$$\hat{S}^\varepsilon_{1,v} = \frac{2}{\gamma^{3/2}\kappa(i\hbar)}[\hat{H}^E(1), (\hat{V}_{U^\epsilon_v})^{1/2}], \tag{5.19}$$

$$\begin{aligned}\hat{S}^{\varepsilon}_{2,v} &= -\sum_{v(\Delta)=v(X)=v}\frac{2^7}{3\gamma^3(i\hbar)^3E(v)}\hat{\phi}(v)\hat{\pi}(v)\\ &\times\ \epsilon(s_Is_Js_K)\epsilon^{IJK}\mathrm{Tr}(\hat{h}_{s_I(\Delta)}[\hat{h}^{-1}_{s_I(\Delta)},(\hat{V}_{U^{\epsilon}_v})^{1/2}]\\ &\times\ \hat{h}_{s_J(\Delta)}[\hat{h}^{-1}_{s_J(\Delta)},(\hat{V}_{U^{\epsilon}_v})^{1/2}]\\ &\times\ \hat{h}_{s_K(\Delta)}[\hat{h}^{-1}_{s_K(\Delta)},(\hat{V}_{U^{\epsilon}_v})^{1/2}]).\end{aligned} \tag{5.20}$$

Note that the family of operators $\hat{H}^{\varepsilon}_{C,\alpha}$ and $\hat{S}^{\varepsilon}_{C,\alpha}$ are cylindrically consistent up to diffeomorphism. Hence the inductive limit operator $\hat{H}_C$ and $\hat{S}_C$ can be densely defined in $\mathcal{H}_G$ by the uniform Rovelli- Smolin topology. Thus we could define master constraint operator $\hat{\mathcal{M}}$ acting on diffeomorphism invariant states as

$$(\hat{\mathcal{M}}\Phi_{Diff})T_{s,c} = \lim_{\mathcal{P}\to\Sigma,\varepsilon,\varepsilon'\to 0}\Phi_{Diff}[\frac{1}{2}\sum_{c\in\mathcal{P}}\left(\hat{H}^{\varepsilon}_C(\hat{H}^{\varepsilon'}_C)^{\dagger}+\hat{S}^{\varepsilon}_C(\hat{S}^{\varepsilon'}_C)^{\dagger}\right)T_{s,c}]. \tag{5.21}$$

Similarly, we can prove that $\hat{\mathcal{M}}$ is a positive and symmetric operator in $\mathcal{H}_{Diff}$ and hence admits a unique self-adjoint Friedrichs extension[6, 36]. Hence it is also possible to obtain the physical Hilbert space of the quantum STT in this special case by the direct integral decomposition of $\mathcal{H}_{Diff}$ with respect to the spectrum of $\hat{\mathcal{M}}$.

VI. COSMOLOGICAL APPLICATION OF QUANTUM BRANS-DIKCE THEORY

For cosmological application of above loop quantum STT, in this section, we will set up the basic structure of loop quantum Brans-Dicke cosmology and get its effective equations of motion [39]. For simplicity, we only consider the spatially flat ($k = 0$) homogeneous and isotropic universe in Brans-Dicke theory. Recall that the original Brans-Dicke theory is the particular case of STT with constant ω and vanishing potential of ϕ. Thus the Hamiltonian constraint of Brans-Dicke theory reads

$$\begin{aligned}H &= \frac{\phi}{2\kappa}\left[F^j_{ab}-(\gamma^2+\frac{1}{\phi^2})\varepsilon_{jmn}\tilde{K}^m_a\tilde{K}^n_b\right]\frac{\varepsilon_{jkl}E^a_kE^b_l}{\sqrt{h}}\\ &+\ \frac{\kappa}{3+2\omega}\left(\frac{(\tilde{K}^i_aE^a_i)^2}{\kappa^2\phi\sqrt{h}}+2\frac{(\tilde{K}^i_aE^a_i)\pi}{\kappa\sqrt{h}}+\frac{\pi^2\phi}{\sqrt{h}}\right)\\ &+\ \frac{\omega}{2\kappa\phi}\sqrt{h}(D_a\phi)D^a\phi+\frac{1}{\kappa}\sqrt{h}D_aD^a\phi.\end{aligned} \tag{6.1}$$

In the cosmological model, classically the metric of spacetime can be written as the following Friedman-Robertson- Walker (FRW) formalism,

$$ds^2 = -dt^2 + a^2(t)[dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi^2)] \tag{6.2}$$

where a is the scale factor. The classical Friedman equation of Brans-Dicke cosmology reads

$$\left(\frac{\dot{a}}{a}+\frac{\dot{\phi}}{2\phi}\right)^2 = \frac{2\omega+3}{12}\left(\frac{\dot{\phi}}{\phi}\right)^2+\frac{8\pi G\rho}{3\phi}. \tag{6.3}$$

Our task is to quantize this model by the loop quantization method and find the quantum dynamical equation as well as its effective expression.

A. Loop quantum Brans-Dicke cosmology

Since the space of our cosmological model is infinite, we introduce an “elemental cell” $\mathcal{V}$ and restrict all integral to $\mathcal{V}$. The homogeneity of the universe guarantee that the whole space information is reflected in this elemental cell. Now we choose a fiducial Euclidean metric ${}^oq_{ab}$ and introduce a pair of fiducial orthnormal triad and co-triad as $({}^oe^a_i, {}^o\omega^i_a)$ respectively such that ${}^oq_{ab} = {}^o\omega^i_a{}^o\omega^i_b$. For simplicity, we let the elemental cell $\mathcal{V}$ be a cubic measured by our fiducial metric and denotes its volume as V_o. Because our FRW metric is spatially flat, we have $\Gamma^i_a = 0$ and hence $A^i_a = \gamma\tilde{K}^i_a$. Via fixing the degrees of freedom of local gauge and diffeomorphism, we finally obtain the connection and densitized triad by symmetrical reduction as [40]:

$$A^i_a = \tilde{c}V_0^{-\frac{1}{3}}{}^o\omega^i_a, \qquad E^b_j = pV_0^{-\frac{2}{3}}\sqrt{\det({}^0q)}{}^oe^b_j, \tag{6.4}$$

where $\tilde{c}$, p are only functions of t. Hence the phase space of the cosmological model consists of conjugate pairs $(\tilde{c}, p)$ and (ϕ, π). The basic Poisson brackets between them can be simply read as

$$\begin{aligned} \{\tilde{c}, p\} &= \frac{\kappa}{3}\gamma, \\ \{\phi, \pi\} &= 1. \end{aligned} \tag{6.5}$$

Note that by the symmetric reduction, the Gaussian and diffeomorphism constraints are satisfied automatically. Also in our homogeneous model, the last two spatial derivative terms in the Hamiltonian constraint (6.1) can be neglected. Hence we only need to consider the first five terms in (6.1). The reduced Hamiltonian in the cosmological model reads

$$H = -\frac{3\tilde{c}^2\sqrt{|p|}}{\gamma^2\kappa\phi} + \frac{\kappa}{(3+2\omega)\phi|p|^{\frac{3}{2}}}(\frac{3\tilde{c}p}{\kappa\gamma} + \pi\phi)^2. \tag{6.6}$$

To quantize the cosmological model, we first need to construct the quantum kinematic of Brans-Dicke cosmology by mimicking the loop quantum STT. This is the so-called polymer-like quantization. The kinematic Hilbert space for the geometry part can be defined as $\mathcal{H}^{\rm gr}_{\rm kin} := L^2(R_{Bohr}, d\mu_H)$, where R_{Bohr} and $d\mu_H$ are respectively the Bohr compactification of the real line and Haar measure on it [40]. On the other hand, for convenience we choose Schrodinger representation for the scalar field [41]. Thus the kinematic Hilbert space for the scalar field part is defined as in usual quantum mechanics, $\mathcal{H}^{\rm sc}_{\rm kin} := L^2(R, d\mu)$. Hence the whole Hilbert space is a direct product, $\mathcal{H}^{total}_{\rm kin} = \mathcal{H}^{\rm gr}_{\rm kin} \otimes \mathcal{H}^{\rm sc}_{\rm kin}$. Now let $|\mu\rangle$ be the eigenstates of $\hat{p}$ in the kinematic Hilbert space $\mathcal{H}^{\rm gr}_{\rm kin}$ such that

$$\hat{p}|\mu\rangle = \frac{8\pi G\gamma\hbar}{6}\mu|\mu\rangle. \tag{6.7}$$

It turns out that those states satisfy the following orthonormal condition

$$\langle\mu_i|\mu_j\rangle = \delta_{\mu_i,\mu_j}\ , \tag{6.8}$$

where δ_{μ_i,μ_j} is the Kronecker delta function rather than the Dirac distribution. For the convenience of studying quantum dynamics, we define new variables

$$v := 2\sqrt{3}\mathrm{sgn}(p)\bar{\mu}^{-3}, \quad b := \bar{\mu}\tilde{c}, \tag{6.9}$$

where $\mathrm{sgn}(p)$ is the sign function for p and $\bar{\mu} = \sqrt{\frac{\Delta}{|p|}}$ with $\Delta = 4\sqrt{3}\pi\gamma\ell_{\rm p}^2$ being a minimum nonzero eigenvalue of the area operator [42]. They also form a pair of conjugate variables as

$$\{b, v\} = \frac{2}{\hbar}. \tag{6.10}$$

It turns out that the eigenstates of $\hat{v}$ also contribute an orthonormal basis in $\mathcal{H}^{\rm gr}_{\rm kin}$. We denote $|\phi, v\rangle$ as the orthogonal basis for the whole Hilbert space $\mathcal{H}^{total}_{\rm kin}$.

Now we come to the quantum dynamics. We treat the first two terms of Hamiltonian constraint (6.1) in the same way as in standard LQC [43]. Hence, the first two terms of the Hamiltonian constraint act on a quantum state $\Psi(v, \phi) \in \mathcal{H}^{total}_{\rm kin}$ as

$$(\hat{H}_1 + \hat{H}_2)\Psi(v,\phi) = \frac{1}{\phi}\left(f_+(v)\Psi(v+4,\phi) + f_0(v)\Psi(v,\phi) + f_-(v)\Psi(v-4,\phi)\right), \tag{6.11}$$

where

$$\begin{aligned} f_+(v) &= \frac{\sqrt{3\Delta}}{16\kappa\gamma^2}\Big||v+3| - |v+1|\Big||v+2|, \\ f_-(v) &= f_+(v-4), \quad f_0(v) = -f_+(v) - f_-(v). \end{aligned} \tag{6.12}$$

Then we turn to the third term $H_3 \equiv \frac{\kappa}{3+2\omega}\frac{(\tilde{K}^i_a E^a_i)^2}{\kappa^2\phi\sqrt{h}}$. Due to spatial flatness, we have $\tilde{K}^i_a E^a_i = \frac{1}{\gamma}A^i_a E^a_i$. In the cosmological model, this term can be reduced by

$$\frac{1}{\gamma}A^i_a E^a_i \rightsquigarrow \frac{3}{\gamma}\tilde{c}p = \frac{3\kappa\hbar b v}{4}. \tag{6.13}$$

Because we use polymer representation for geometry, their is no quantum operator corresponding to connection $\tilde{c}$ as in standard LQC [41]. Hence we have to replace the connection by holonomy to get a well-defined operator. It turns out that the term H_3 can be quantized, and its action on a quantum state reads [39]

$$\begin{aligned}\hat{H}_3\Psi(\phi,v) &= \frac{2\sqrt{3}\kappa}{\beta\phi(\Delta)^{\frac{3}{2}}}\left(\frac{3\hbar}{4}\right)^2\sin(b)\hat{|v|}\sin(b)\Psi(\phi,v)\\ &= -\frac{\sqrt{3}\kappa}{2\beta\phi(\Delta)^{\frac{3}{2}}}\left(\frac{3\hbar}{4}\right)^2\left[|v+2|\Psi(\phi,v+4)-2|v|\Psi(\phi,v)+|v-2|\Psi(\phi,v-4)\right],\end{aligned}\tag{6.14}$$

where we set $\beta = 3+2\omega$. Similarly, the fourth term $H_4 \equiv \frac{2\kappa}{3+2\omega}\frac{(\tilde{K}^i_a E^a_i)\pi}{\kappa\sqrt{h}}$ can also be quantized, and its action on a wave function reads

$$\begin{aligned}\hat{H}_4\Psi(\phi,v) &= \frac{2\sqrt{3}\kappa}{\beta(\Delta)^{\frac{3}{2}}}\left(\frac{3\hbar}{4}\right)2\mathrm{sgn}(p)\sin(b)\hat{\pi}\Psi(\phi,v)\\ &= \frac{2\sqrt{3}\kappa}{\beta(\Delta)^{\frac{3}{2}}}\left(\frac{3\hbar}{4}\right)\hbar\mathrm{sgn}(p)[\frac{\partial\Psi(\phi,v+2)}{\partial\phi}-\frac{\partial\Psi(\phi,v-2)}{\partial\phi}].\end{aligned}\tag{6.15}$$

The last term $H_5 \equiv \frac{\kappa}{3+2\omega}\frac{\pi^2\phi}{\sqrt{h}}$ can be quantized as

$$\begin{aligned}\hat{H}_5\Psi(\phi,v) &= \frac{2\sqrt{3}\kappa}{\beta(\Delta)^{\frac{3}{2}}}\widehat{|v|^{-1}}(\hat{\pi})\hat{\phi}\hat{\pi}\Psi(\phi,v)\\ &= -\frac{2\sqrt{3}\kappa}{\beta(\Delta)^{\frac{3}{2}}}(\hbar)^2B(v)\phi\frac{\partial^2\Psi(\phi,v)}{\partial\phi^2},\end{aligned}\tag{6.16}$$

where

$$B(v) = (\frac{3}{2})^3|v|\Big||v+1|^{1/3}-|v-1|^{1/3}\Big|^3.\tag{6.17}$$

The total Hamiltonian constraint equation of loop quantum Brans-Dicke cosmology reads

$$(\sum_{i=1}^{5}\hat{H}_i)\Psi(\phi,v) = 0.\tag{6.18}$$

B. Effective equation

To study the effective theory of loop quantum Brans-Dicke cosmology, we also want to know the effect of matter fields on the dynamical evolution. Hence we include an extra massless scalar matter field φ into Brans-Dicke cosmology. Then classically the total Hamiltonian constraint of the model reads

$$H = -\frac{3\tilde{c}^2\sqrt{|p|}}{\gamma^2\kappa\phi}+\frac{\kappa}{(3+2\omega)\phi|p|^{\frac{3}{2}}}(\frac{3\tilde{c}p}{\kappa\gamma}+\pi\phi)^2+\frac{p_\varphi^2}{2|p|^{\frac{3}{2}}},\tag{6.19}$$

where p_φ is the momentum conjugate to φ. The effective description of LQC is a delicate and topical issue since it may relate the quantum gravity effects to low-energy physics. The effective equations of LQC are being studied from both canonical perspective[44–47] and path integral perspective[48–52]. Since the key element in the polymer-like quantization of previous subsection is to take holonomies rather than connections as basic variables, a heuristic and simple way to get the effective equations is to do the replacement $\tilde{c} \to \frac{\sin(\bar{\mu}\tilde{c})}{\bar{\mu}}$ or $b \to \sin b$. Under this replacement, the effective version of Hamiltonian constraint (6.19) takes the form

$$H = -\frac{3\sin^2(\bar{\mu}\tilde{c})\sqrt{|p|}}{\kappa\gamma^2\phi\bar{\mu}^2}+\frac{\kappa}{\beta\phi|p|^{\frac{3}{2}}}(\frac{3\sin(\bar{\mu}\tilde{c})p}{\bar{\mu}\kappa\gamma}+\pi\phi)^2+|p|^{\frac{3}{2}}\rho,\tag{6.20}$$

where $\rho=\frac{p_\varphi^2}{2|p|^3}$ by definition is the matter density. It is worth noting that the effective Hamiltonian (6.20) can also be derived by a path integral formalism [39]. Then the canonical equations of motion read

$$\dot{p} = \frac{2\sqrt{|p|}}{\gamma\phi\bar{\mu}}\sin(\bar{\mu}\tilde{c})\cos(\bar{\mu}\tilde{c}) - \frac{2\kappa}{\beta\phi|p|^{\frac{1}{2}}}\mathrm{sgn}(p)\left(\frac{3\sin(\bar{\mu}\tilde{c})p}{\bar{\mu}\kappa\gamma}+\pi\phi)\cos(\bar{\mu}\tilde{c}\right), \tag{6.21}$$

$$\dot{\phi} = \frac{2\kappa}{\beta|p|^{\frac{3}{2}}}(\frac{3\sin(\bar{\mu}\tilde{c})p}{\bar{\mu}\kappa\gamma}+\pi\phi). \tag{6.22}$$

In the above calculation, the Poisson brackets (6.5) were used. The Combination of equations (6.21) and (6.22) gives

$$\begin{aligned}\left(\frac{\dot{p}}{2p}+\frac{\dot{\phi}}{2\phi}\right)^2 &= \left[\frac{\mathrm{sgn}(p)}{\gamma\phi\bar{\mu}\sqrt{|p|}}\sin(\bar{\mu}\tilde{c})\cos(\bar{\mu}\tilde{c})+\frac{\kappa}{\beta\phi|p|^{\frac{3}{2}}}(\frac{3\sin(\bar{\mu}\tilde{c})p}{\bar{\mu}\kappa\gamma}+\pi\phi)(1-\cos(\bar{\mu}\tilde{c}))\right]^2\\ &= \left[\frac{\mathrm{sgn}(p)}{\gamma\phi\sqrt{\Delta}}\sin(\bar{\mu}\tilde{c})\cos(\bar{\mu}\tilde{c})+\frac{\dot{\phi}}{2\phi}(1-\cos(\bar{\mu}\tilde{c}))\right]^2.\end{aligned} \tag{6.23}$$

On the other hand, from effective Hamiltonian constraint (6.20) we can get

$$-\frac{3\sin^2(\bar{\mu}\tilde{c})}{\kappa\gamma^2\phi\Delta}+\frac{\beta\dot{\phi}^2}{4\kappa\phi}+\rho=0, \tag{6.24}$$

which implies

$$\sin^2(\bar{\mu}\tilde{c})=\frac{\rho_{eff}}{\rho_c}, \tag{6.25}$$

where $\rho_c=\frac{3}{\gamma^2\Delta\kappa}=\frac{\sqrt{3}}{32\pi^2G^2\gamma^3\hbar}$ and $\rho_{eff}=\frac{\beta\dot{\phi}^2}{4\kappa}+\phi\rho$. Taking account of Eq. (6.25), we can rewrite Eq. (6.23) as

$$\left(\frac{\dot{a}}{a}+\frac{\dot{\phi}}{2\phi}\right)^2 = \left[\frac{1}{\phi}\sqrt{\frac{\kappa}{3}\rho_{eff}(1-\frac{\rho_{eff}}{\rho_c})}+\frac{\dot{\phi}}{2\phi}(1-\sqrt{1-\frac{\rho_{eff}}{\rho_c}})\right]^2. \tag{6.26}$$

This is the effective Friedmann equation of Brans-Dicke cosmology, which contains important quantum correction terms. In addition, we can show that for a contracting universe, ρ_{eff} monotonically increase while v decreases[39]. Thus it is easy to see from Eq.(6.26) that, when ρ_{eff} approaches ρ_c, one gets $\cos(\bar{\mu}\tilde{c})=1-\frac{\rho_{eff}}{\rho_c}=0$. Then from Eq. (6.21), we can obtain $\dot{p}=0$. This implies a quantum bounce would happen at that point for a contracting universe.

We end up this section with several remarks. First, when $\phi=1$, because of $\rho_{eff}=\rho$ and $\dot{\phi}=0$ we would return to the well-known effective Friedmann equation of LQC [43, 45] as

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{\kappa}{3}\rho(1-\frac{\rho}{\rho_c}). \tag{6.27}$$

Second, when $\rho_{eff}\ll\rho_c$, we can omit $\frac{\rho_{eff}}{\rho_c}$ terms in Eq. (6.26) to get the classical limit of this equation as

$$\begin{aligned}\left(\frac{\dot{a}}{a}+\frac{\dot{\phi}}{2\phi}\right)^2 &= \frac{1}{\phi^2}\frac{\kappa}{3}\rho_{eff}=\frac{\kappa}{3\phi^2}(\frac{\beta\dot{\phi}^2}{4\kappa}+\phi\rho)\\ &= \frac{\beta\dot{\phi}^2}{12\phi^2}+\frac{\kappa\rho}{3\phi},\end{aligned} \tag{6.28}$$

which is nothing but the classical Friedmann equation of Brans-Dicke cosmology. Hence the effective theory has correct classical limit.

VII. CONCLUSION AND OUTLOOK

Modified gravity has received increased attention in issues of “dark matter”, “dark energy” and nontrivial tests on gravity beyond GR. Some kinds of modified gravity theories have also become popular in certain unification schemes such as string theory. Whether some modified gravity theories could be nonperturbatively quantized is certainly an interesting and challenging

question. In this review, as an example, we first set up the $su(2)$-connection dynamical formalism of STT. Then LQG method has been successfully extended to the STT by coupling to a polymer-like scalar field. This successful extension strongly hints that the nonperturbative quantization procedure might be valid even for more general modified gravity theories. At least, as we demonstrated, loop quantization procedure should be valid for any metric theories with a well-defined geometrical dynamics. Hence it is desirable to study the Hamiltonian formulation of modified gravity theories and try to cast those theories into the $su(2)$-connection dynamical formalism. Then, we can naturally extend nonperturbative loop quantization method to those theories.

The concrete results of this paper are summarized as follows. A general loop quantization scheme for metric modified gravity is first given in section II. Then we use STT as an example to show how our general procedure works. By doing Hamiltonian analysis, we have successfully derived the Hamiltonian formulation of STT of gravity from their Lagrangian formulation. The result shows that these theories can be naturally divided into two different sectors by the coupling parameter $\omega(\phi)$. In the first sector of $\omega(\phi) \neq -3/2$, the resulted canonical structure and constraint algebra of STT are similar to those of GR minimally coupled with a scalar field. While in the sector of $\omega(\phi) = -3/2$, the feasible theories are strongly restricted and a new primary constraint which generating conformal transformations of spacetime is obtained. The corresponding canonical structure and constraint algebra are also obtained. It is worth noting that the Palatini $f(\mathcal{R})$ theories are equivalent to this sector of STT. The successful background independent LQG relies on the key observation that GR can be cast into the $su(2)$-connection dynamics. We have shown that the connection dynamical formalism of the STT can also be obtained by canonical transformations from the geometrical dynamics. Based on the connection dynamical formalism with structure group $SU(2)$, loop quantization method has been successfully extended to the STT by coupling to a polymer-like scalar field. The quantum kinematical structure of STT is as same as that of loop quantum gravity coupled with a scalar field. Thus the important physical result that both the area and the volume are discrete at kinematic level remains valid for quantum STT of gravity. While the dynamics of STT is more general than that of LQG, the Hamiltonian constraint operators and master constraint operators for STT can also be well defined in both sectors respectively. In particular, in the sector $\omega(\phi) = -3/2$, the extra conformal constraint can also be promoted as a well-defined operator. Hence the classical STT in both sectors have been successfully quantized non-perturbatively. This ensures the existence of the STT of gravity at fundamental quantum level. As the cosmological application of the above loop quantum STT, we construct a particular type of loop quantum scalar-tensor cosmology, which is the so-called Brans-Dicke cosmology. For simplicity, we only restrict ourselves to the sector of $\omega \neq -\frac{3}{2}$. It turns out that the classical differential equation of Brans-Dicke cosmology, which represents the cosmological evolution, is now replaced by quantum difference equation. The effective Friedmann equation of loop quantum Brans-Dicke cosmology is also given, which shows that the classical big bang singularity is again replaced by a quantum bounce. This effective equation lays a foundation for further phenomenological investigation to possible quantum gravity effects in Brans-Dicke cosmology.

It should be noted that there are still many aspects of the connection formalism and loop quantization of modified gravity, which deserve discovering. Taking STT for examples, it is still desirable to derive the connection dynamics of STT by variational principle. The semiclassical analysis of loop quantum STT is yet to be done. In our loop quantum Brans-Dicke cosmology, some phenomenological issues, such as inflation, would be studied in future works. To further explore the physical contents of the loop quantum STT, we would also like to study its applications to black holes in future works. In addition, one would also like to quantize STT via the covariant spin foam approach. Furthermore, nonperturbative loop quantization of other types of modified gravity, such as Horava-Lifshitz theory and critical gravity etc, is also desirable.

Acknowledgments

This work is supported by NSFC (Grant No.10975017, No.11235003 and No.11275073) and the Fundamental Research Funds for the Central Universities under Grant No.2012ZZ0079.

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